Phenol, 3-methoxy-5-(2-phenylethyl)-17635-59-5 | DTXSID80170114

Model Performance

| Model | Data |
|-------|------|
| Model | Dala |
| | |

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.95 | 0.69 | 0.95 | 0.65 | 0.96 | 0.68 |

Model Results

Predicted value: 9.83

Global applicability domain: Outside

Local applicability domain index: 7.94e-01

Confidence level: 3.81e-01

Nearest Neighbors from the Training Set

Image not found

1-Hexadecanol Measured: 9.90 Predicted: 9.79 Image not found

Diphenylamine Measured: 7.64 Predicted: 8.73 Image not found

1-Octadecanol Measured: 10.9 Predicted: 10.5

Image not found

Phenacetin Measured: 9.59 Predicted: 9.23 Image not found

1-Eicosanol Measured: 12.1 Predicted: 11.2